Discrete Mathematics 311 (2011) 2233–2237

Contents lists available at SciVerse ScienceDirect

Discrete Mathematics

journal homepage: www.elsevier.com/locate/disc

On the differences between Szeged and Wiener indices of graphs

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ARTICLE INFO

Article history:
Received 28 December 2010
Received in revised form 16 June 2011
Accepted 17 June 2011
Available online 31 July 2011

Keywords:
Szeged index
Wiener index
Block

ABSTRACT

Let G be a connected graph and $\eta(G) = Sz(G) - W(G)$, where $W(G)$ and $Sz(G)$ are the Wiener and Szeged indices of G, respectively. A well-known result of Klavžar, Rajapakse, and Gutman states that $\eta(G) \geq 0$, and by a result of Dobrynin and Gutman $\eta(G) = 0$ if and only if each block of G is complete. In this paper, a path-edge matrix for the graph G is presented by which it is possible to classify the graphs in which $\eta(G) = 2$. It is also proved that there is no graph G with the property that $\eta(G) = 1$ or $\eta(G) = 3$. Finally, it is proved that, for a given positive integer k, $k \neq 1, 3$, there exists a graph G with $\eta(G) = k$.

1. Introduction

Throughout this article, G is a simple connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, the distance between vertices u and v of G is denoted by $d_G(u, v)$ ($d(u, v)$ for short), and it is defined as the number of edges in a minimal path connecting them. The eccentricity of a vertex x is defined as $\varepsilon_G(x) = max\{d(x, y) \mid y \in V(G)\}$. A subgraph H of a graph G is called isometric, and we write $H \ll G$, if $d_H(x, y) = d_G(x, y)$, for each unordered pair $\{x, y\}$ of vertices in H.

A topological index is a numerical quantity related to a graph that is invariant under graph isomorphisms. A topological index related to the distance function $d(-, -)$ is called a "distance-based topological index". The Wiener index $W(G)$ was the first distance-based topological index; it is defined as the sum of all distances between vertices of G [17]. The Wiener index has noteworthy applications in chemistry, and interested readers are referred to [2,3] and the references therein for the mathematical properties and chemical meaning of this index. Hosoya [6] was the first scientist to introduce the name "topological index", and to reformulate the Wiener index in terms of the distance function $d(-, -)$.

We now describe some notation which will be kept throughout. Suppose that $e = uv$. Define $n_u(e)$ to be the number of vertices of G lying closer to u than v; $n_v(e)$ is defined analogously. The Szeged index of G is defined as $Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e)$. Notice that vertices equidistant from both ends of the edge $e = uv$ are not counted. This topological index is a mathematically elegant topological index, defined by Gutman [7]. We encourage readers to consult [1,19–21] for computational techniques and [8–10,12,14,18] for mathematical properties of this topological index.

Lukovits [13] introduced an all-path version of the Wiener index. To explain, we assume that G is a connected graph with $V(G) = \{1, 2, \ldots, n\}$. Then $P(G) = \sum_{i<j} \sum_{P\in\pi_{i,j}} |P|$ is called the "all-path" version of the Wiener index. Here, $\pi_{i,j}$ denotes the set of all paths connecting vertices i, j, and the summations have to be performed between all pairs of vertices i and j and for all paths between i and j. In the paper mentioned, some mathematical properties of $P(G)$ together with its extremal values are investigated. In the next section, we present an "path-edge" matrix to study the Wiener and Szeged indices of a graph, simultaneously. This matrix is defined in a similar way as the "all-path" matrix of Lukovits.

Throughout this paper, our notation is standard, and is taken mainly from [15,16]. We let K_n, P_n, and C_n denote the complete graph, path, and cycle on n vertices, respectively. The length of a path P is denoted by $|P|$. Suppose that G is a

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doi:10.1016/j.disc.2011.06.019

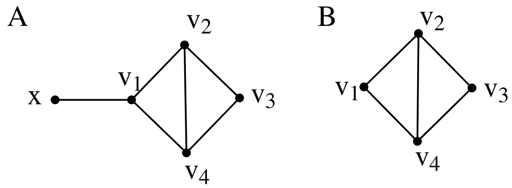

Fig. 1. The graphs A and B.

connected graph and $e = uv \in E(G)$. Define

$$N_u(e) = \{x \in V(G) \mid d(x,u) < d(x,v)\},$$
$$N_v(e) = \{x \in V(G) \mid d(x,u) > d(x,v)\},$$
$$N_0(e) = \{x \in V(G) \mid d(x,u) = d(x,v)\}.$$

Thus $n_u(e) = |N_u(e)|$ and $n_v(e) = |N_v(e)|$. A set $Y = \{P_1, P_2, \ldots, P_{\binom{n}{2}}\}$ of shortest paths in G such that for every vertex $a, b \in V(G)$, $a \neq b$, there exists a unique path $P \in Y$ connecting vertices a and b is called a complete set of shortest paths of G (CSSP for short). Define the matrix $A_Y = [a_{ij}^Y]$, as follows:

$$a_{ij}^Y = \begin{cases} 1 & e_j \in E(P_i) \\ 0 & e_j \notin E(P_i). \end{cases}$$

Clearly, if P_i is a path connecting vertices x and y then $d(x, y)$ is the number of non-zero entries in the ith row of A_Y. Thus the summation of entries of the matrix A_Y is equal to the Wiener index of G. In what follows, $P_G(u, v)$ denotes the set of all shortest paths connecting vertices u and v of G and CSSP(G) denotes the set of all CSSPs of G.

For the sake of completeness, we mention below two results of [11], which are crucial throughout the paper.

Lemma 1. *Suppose that $e = uv \in E(G)$ and that a and b are arbitrary vertices of G. If there exists $P \in P_G(a, b)$ such that $e \in E(P)$, then one of the following is satisfied:*

(i) *$a \in N_u(e)$ and $b \in N_v(e)$,*
(ii) *$a \in N_v(e)$ and $b \in N_u(e)$.*

Lemma 2. *Suppose that G is a graph containing a non-complete block. Then the following are satisfied.*

(i) *The graph G has an induced subgraph isomorphic to $K_4 - e$ or cycle C_n, $n \geq 4$.*
(ii) *If G does not have an induced subgraph isomorphic to $K_4 - e$ then, in the smallest induced cycle C_n, $n \geq 4$, the following condition is satisfied:*

$$\forall x, y \in V(C) : d_C(x, y) = d_G(x, y).$$

2. Main results

Let G be a connected graph. A maximal 2-connected subgraph of G is called a block of G. The block graphs are connected graphs in which every block is a clique. The block tree of G is a tree T such that the vertices of T correspond to the blocks and cut vertices of G. The edges of T are those connecting a cut vertex v to a block B such that $v \in V(B)$.

In [4], Dobrynin and Gutman investigated the structure of a connected graph G with the property that $Sz(G) = W(G)$. They conjectured that $Sz(G) = W(G)$ if and only if G is a block graph. This conjecture was proved by the same authors [5] one year after proposing it. The motivation of this paper comes from this.

Suppose that G is an n-vertex and m-edge graph with the path-edge matrix A_Y, $Y \in CSSP(G)$, and that H is an isometric subgraph of G. It is clear that $|Y| = \binom{n}{2}$. If $e = uv$ is an edge of H, then we define $\eta_Y^G(e_j) = n_u(e_j)n_v(e_j) - \sum_i a_{ij}^Y$, $1 \leq j \leq m$, and $\eta_Y^G(H) = \sum_{e \in E(H)} \eta_Y^G(e)$. If $H = G$, then we write $\eta_Y(G)$ instead of $\eta_Y^G(G)$. Notice that $\eta_Y^H(H) \leq \eta_Y^G(H)$, and it is far from true that $\eta_Y^H(H) = \eta_Y^G(H)$. To do this, we consider the following example.

Example 3. Suppose that A and B are the graphs depicted in Fig. 1. Clearly, $\eta(B) = 2$. Choose a vertex x adjacent to v_1 in A, $f_1 = v_1v_4$, and $f_2 = v_3v_4$. Then $x \in N_{v_1}(f_1)$ and $v_3 \in N_{v_4}(f_1)$. There are two shortest paths connecting v_1 and v_3, as well as for x and v_3. So, by choosing a suitable set $Y \in CSSP(G)$, one can see that $\eta_Y^A(f_1) = 2$. On the other hand, the fact that $x, v_1 \in N_{v_4}(f_2)$ implies that there are two shortest paths connecting x, v_3 and two shortest paths between v_1, v_3. Therefore, $\eta_Y^A(f_2) = 2$, and so $\eta_Y^A(A) = 4$.

It is easy to see that $\eta_Y(G) = Sz(G) - W(G)$, and so the value of $\eta_Y(G)$ is independent of Y. So, we can write $\eta(G)$ as $\eta_Y(G)$.

Lemma 4. *Let G be a connected graph, and let B be a block of G. Then, for each $Y, Z \in CSSP(G)$, $\eta_Y^G(B) = \eta_Z^G(B)$.*

Proof. By definition,

$$\eta_Y^G(B) - \eta_Z^G(B) = \sum_{e_j \in E(B)} \left[\eta_Y^G(e_j) - \eta_Z^G(e_j)\right]$$
$$= \sum_{e_j = uv \in E(B)} \left[\left(n_u(e_j)n_v(e_j) - \sum_i a_{ij}^Y\right) - \left(n_u(e_j)n_v(e_j) - \sum_i a_{ij}^Z\right)\right]$$
$$= \sum_j \sum_i a_{ij}^Y - \sum_j \sum_i a_{ij}^Z = 0,$$

proving the lemma. □

It is obvious that if $H \ll G$ and $Y \in CSSP(G)$ then $\eta_Y^G(H) \geq \eta(H)$.

Lemma 5. *Suppose that G is a connected graph and that H is an isometric subgraph of G isomorphic to $K_4 - e$. Then $\eta(G) \geq 2$.*

Proof. Suppose $V(H) = \{v_1, v_2, v_3, v_4\}$ such that v_1 and v_3 are not adjacent. Since $H \ll G$, without loss of generality, assume that $P : v_1v_2v_3$ is a shortest path of Y connecting v_1 and v_3. Suppose that $e_1 = v_1v_4$ and $e_2 = v_3v_4$. Then $v_1 \in N_{v_1}(e_1)$ and $v_3 \in N_{v_4}(e_1)$, while the shortest path of Y connecting v_1 and v_3 is not through the edge e_1. Therefore, $\eta_Y^G(e_1) \geq 1$. Using a similar argument, one can prove that $\eta_Y^G(e_2) \geq 1$. Since $\eta(G) \geq \eta_Y^G(H) \geq 2$, the proof is complete. □

Suppose that A and B are subgraphs isomorphic to $K_4 - e$ in a graph G, that D_A is the set of all vertices of degree 2 in A, and that D_B is defined analogously. The subgraphs A and B are said to be distinct if $D_A \neq D_B$.

Corollary 6. *Suppose that G has exactly k mutually distinct subgraphs isomorphic to $K_4 - e$. Then*

(1) $\eta(G) \geq 2k$,
(2) $\eta(K_n - e) \geq 2(n - 3)$.

Proof. The proof is straightforward, and it is omitted. □

Lemma 7. *Suppose that G is a connected graph containing an induced cycle C of length n, $n \geq 4$. Then the following hold.*

(i) *If C is an isometric cycle of a block B of G, then $\eta(G) \geq \eta_Y^G(B) \geq \eta_Y^G(C) \geq n$.*
(ii) *If C is a minimal induced cycle of a block B of G, then $\eta(G) \geq \eta_Y^G(B) \geq n$.*

Proof. Suppose that the block B contains an isometric cycle C on n vertices with $V(C) = \{v_1, v_2, \ldots, v_n\}$.

(i) For each i, j, $d_G(v_i, v_j) = d_C(v_i, v_j)$. Choose $e_t = v_1v_2 \in V(C)$, $1 \leq t \leq |E(G)|$, and n to be even. Then $v_{1+\frac{n}{2}} \in N_{v_2}(e_t)$, $v_{2+\frac{n}{2}} \in N_{v_1}(e_t)$, and there is no shortest path connecting $v_{1+\frac{n}{2}}$ and $v_{2+\frac{n}{2}}$ which contains e_t. This implies that, if $A_Y = [a_{ij}^Y]$ and $P_r \in Y$ is a shortest path connecting $v_{1+\frac{n}{2}}$ and $v_{2+\frac{n}{2}}$, then $a_{rt}^Y = 0$. Therefore, $\eta_Y^G(e_t) \geq 1$. If n is odd, then similarly $v_{\frac{n+1}{2}+1} \in N_{v_1}(e_t)$, $v_{\frac{n-1}{2}+1} \in N_{v_2}(e_t)$, and the shortest path of Y connecting $v_{\frac{n-1}{2}+1}$ and $v_{\frac{n+1}{2}+1}$ does not pass the edge e_t. Thus $\eta_Y^G(e_t) \geq 1$. Since $C \ll B \ll G$, by the arguments of the paragraph before Example 3, $\eta(G) \geq \eta_Y^G(B) \geq \eta_Y^G(C) \geq n$, which concludes the result.

(ii) Assume that block B contains a minimal induced cycle C on n vertices. If C is isometric, there is nothing to prove. If C is not isometric, then there exist i, j such that $d_G(v_i, v_j) < d_C(v_i, v_j)$. Without loss of generality, we can assume that the shortest path of Y connecting v_i and v_j does not cross $V(C) - \{v_i, v_j\}$. Consider two incident edges $f_1 = v_{k-1}v_k$ and $f_2 = v_kv_{k+1}$, $k \neq i$. Since C is induced cycle, it does not have a chord, and so v_{k-1} and v_{k+1} are not adjacent. Suppose that C' is the shortest cycle containing f_1 and f_2. Obviously, $C' \neq C$, and C' is not an induced cycle. So, it has a chord, say f. If v_k is not an endpoint of f, then we shall find a cycle smaller than C' containing f_1 and f_2, which is impossible. Thus, v_kx is a chord of C'. Look at the cycle $v_kv_{k+1}\cdots xv_k$. Since every chord of C' is incident to v_k and C is a minimal induced cycle of B, v_k is adjacent to every vertex of C'. This shows that each of the edges f_1 and f_2 is at least contained in an isometric subgraph isomorphic to $K_4 - e$. Therefore, by Corollary 6, $\eta(G) \geq \eta_Y^G(B) \geq n$. □

Lemma 8. *Suppose that G is a connected graph and that $Y \in CSSP(G)$. If $\eta_Y^G(e_j) > 0$, then e_j is contained in an induced subgraph isomorphic to $K_4 - e$ or an induced cycle C_n, $n \geq 4$.*

Proof. Suppose that $\eta_Y^G(e_j) > 0$, $Y \in CSSP(G)$, and $A_Y = [a_{ij}^Y]$. Then there exists j such that $\sum_i a_{ij} < n_u(e_j)n_v(e_j)$, where $e_j = uv$. This means that we can choose $a \in N_u(e_j)$, $b \in N_v(e_j)$ such that $e_j \notin P_{(a,b)}$, where $P_{(a,b)}$ is the unique path of Y connecting a and b. Our main proof considers three separate cases, as follows.

Case 1. *$a = u$ and $b \neq v$.* Suppose that Q is a shortest path connecting b and v. If x is the first common vertex of $P_{(a,b)}$ and Q in traversing from v to b, then $x \in N_v(e_j)$. Since $e_j = uv \notin P_{(a,b)}$, $x \neq v$. So, $d(x, v) \geq 1$, $d(x, u) \geq 2$, and the length of the cycle C through x, u, and v is at least 4. Let $u_1 \neq v$ be the vertex adjacent to u in C. It is clear that u_1 is not adjacent to v. Assume that C' is a shortest cycle containing edges uu_1 and uv. If C' is an isometric cycle, then, by Lemma 7, the proof is complete. Otherwise, by similar arguments to those are given in the second part of Lemma 7, we can prove that uv is an edge of an induced subgraph isomorphic to $K_4 - e$.

Case 2. $a \neq u$ *and* $b = v$. It is enough to apply a similar argument to those given in Case 1.

Case 3. $a \neq u$ *and* $b \neq v$. Consider Q_1 and Q_2 to be the shortest paths connecting a, u and b, v, respectively. Suppose that $x \in V(Q_1) \cap V(Q_2)$ and $d(x, u) \leq d(x, v)$. Then $d(b, u) \leq d(b, x) + d(x, u) \leq d(b, x) + d(x, v) = d(b, v)$, and so $b \notin N_v(e_j)$, a contradiction. If $x \in V(Q_1) \cap V(Q_2)$ and $d(x, u) > d(x, v)$, then $d(a, v) \leq d(a, x) + d(x, v) < d(a, x) + d(x, u) = d(a, u)$, and so $a \in N_v(e_j)$, which leads to another contradiction. Therefore, $V(Q_1) \cap V(Q_2) = \emptyset$. Suppose that x is the last common vertex of $P_{(a,b)}$ and Q_1 and that y is the first common vertex of $P_{(a,b)}$ and Q_2 in traversing the path $P_{(a,b)}$ from a to b. By our assumption, $d(x, y) \geq 1$. If $x = u$, then $v \notin V(P_{(a,b)})$, and if $y = v$, then $x \neq u$. In each case, a similar argument to that of Cases 1 or 2 shows that e is contained in an induced subgraph isomorphic to $K_4 - e$ or C_n, $n \geq 4$. Therefore, we can assume that $x \neq u$ and $y \neq v$. Consider the cycle C containing x, u, v, and y, and apply the end part of Case 1. This completes our proof. □

Lemma 9. *Suppose that G is a connected graph and that B is a block of G such that B does not have C_n, $n \geq 4$, as an induced subgraph. Then, for each $Y \in CSSP(G)$ and $f = uv \in E(B)$, $\eta_Y^G(f) = 0$ if and only if, for every vertex $x \neq u, v$ of B, $d(x, u) = d(x, v)$. In particular, if B is complete then $\eta_Y^G(B) = 0$.*

Proof. Suppose that, for each vertex $x \in V(B)$, x is equidistant from the end of $f = uv$. To prove that $\eta_Y^G(f) = 0$, we have to show that, for every $z \in N_u(f)$ and $z' \in N_v(f)$, the shortest path between z and z' is through the edge f. If u and v are not cut vertices of G, then $N_u(f) = \{u\}$ and $N_v(f) = \{v\}$. So, $\{z, z'\} = \{u, v\}$, and it is enough to choose f as the shortest path connecting u and v. If u or v, say u, is a cut vertex, then, by considering u as the root of the block tree of G, one can see that all vertices other than those that are in the branch corresponding to B belong to $N_u(f)$. The same is true when v is a cut vertex of G. Since u or v is a cut vertex of G, for each $z \in N_u(f)$ and $z' \in N_v(f)$, the shortest path between z and z' is through the edge f, as desired.

Conversely, assume that for every $Y \in CSSP(G)$ there exists $f = uv \in E(B)$ such that $\eta_Y^G(f) = 0$ and $d(x, u) < d(x, v)$, for some $x \in V(B)$. Suppose that $P : u, u_1, u_2, \ldots, u_r, x$ is a shortest path connecting u, x and $Q : v, v_1, v_2, \ldots, v_s, x$ is a path in B between v and x such that $u \notin V(Q)$. Clearly, u_1 and v are not adjacent. Look at the incident edge uu_1 and uv of B. Since B does not have an induced cycle C_n, $n \geq 4$, by using a similar argument to that given in the proof of Lemma 7(ii), one can show that the edge uv is an edge of an induced subgraph isomorphic to $K_4 - e$. Thus we can choose Y such that $\eta_Y^G(f) > 0$, which completes our lemma. □

Let G be a graph, and let $a \in V(G)$ be a fixed vertex. Define $A_i^G(a)$ (A_i for short) to be the set of all vertices having distance i from a. Then for each edge $e \in E(G)$ there exists i, $1 \leq i \leq \varepsilon(a)$, such that e connects a vertex of $A_i^G(a)$ to another vertex of $A_j^G(a)$, $j = i$ or $j = i + 1$.

Lemma 10. *Let G be a graph, and let B be a block of G. Then, for each $Y \in CSSP(G)$, $\eta(B) = \eta_Y^G(B)$ if and only if cut vertices of G in B are adjacent to all vertices of B.*

Proof. ($\Longleftarrow$) The proof is similar to that given in the first part of the proof of Lemma 9.

($\Longrightarrow$) We assume that, for each $Y \in CSSP(G)$, $\eta(B) = \eta_Y^G(B)$, and that there exists a cut vertex $x \in V(B)$ and a vertex $y \in V(B)$ such that $d(x, y) \geq 2$. We claim that there exists an edge $f \in E(B)$ such that $\eta_Y^B(f) < \eta_Y^G(f)$. To prove this, we consider the vertex x as a root for B and choose $f = uv$, where $u \in A_{k-1}^B(x)$, $v \in A_k^B(x)$ and $k = \varepsilon_B(x)$. It is obvious that $x \in N_u(f)$. If there exists a vertex $z \in V(B)$ such that z is adjacent to v and not adjacent to u, then $z \in N_v(f)$, and it is possible to find a shortest path P connecting x and z, where $uv \notin E(P)$. Choose an arbitrary vertex z' in a block B' containing x different from B. Then $z' \in N_u(f)$, and we can find a shortest path P' between z and z' with $uv \notin P'$. Thus, we can choose the set Y such that $\eta_Y^B(f) < \eta_Y^G(f)$. If there is no such a vertex z, then $v \in N_v(f)$. Now, if v is adjacent to a vertex of $A_{k-1}^B(x)$ other than u, then it is possible to find a shortest path P_1 connecting v and z' such that $uv \notin P_1$. So, one can choose the set Y such that $\eta_Y^B(f) < \eta_Y^G(f)$. Otherwise, v is adjacent to a vertex w in $A_k^B(x)$. Suppose that $w' \neq u \in A_{k-1}^B(x)$ is a vertex adjacent to w. Consider the edge ww', and repeat our argument to construct a set Y to lead to our final contradiction. □

Theorem 11. *There is no graph G with $\eta(G) = 1$.*

Proof. Suppose that G is a connected graph with $\eta(G) = 1$. By [5, Proposition 3] and Lemma 2(i), G contains an induced subgraph isomorphic to $K_4 - e$ or C_n, $n \geq 4$. We now apply Lemmas 5 and 7 to prove that $\eta(G) \geq 2$, a contradiction. □

Suppose that $\mathcal{K}_2$ denotes the set of all graphs containing one – exactly one – non-complete block, say B, where $B \cong K_4 - e$ and vertices of degree 2 of B are not cut vertices of G.

Theorem 12. $\eta(G) = 2$ *if and only if* $G \in \mathcal{K}_2$.

Proof. If $G \in \mathcal{K}_2$ then, by Lemmas 9 and 10, $\eta(G) = 2$. Suppose that $\eta(G) = 2$. Then, by [5, Proposition 3] and Lemmas 2(i) and 7, G does not have induced subgraph isomorphic to C_n, $n \geq 4$. Thus, G has an induced subgraph H isomorphic to $K_4 - e$. Suppose that B is a block of G containing H. Since $\eta(G) \geq \eta(H) = 2$, for each $Y \in CSSP(G)$ and for each edge $f \in E(G) - E(H)$ we have $\eta_Y^C(f) = 0$. By Lemma 9, if $x \in V(B) - V(H)$ is adjacent to at least one vertex of H, then, by Lemma 10, x is adjacent to each vertex of H. We now apply Corollary 6 to deduce that $\eta(G) \geq \eta(B) \geq 4$, which is impossible. Thus $H \cong B$. Since $\eta(H) = \eta(B) = 2$, by Lemmas 2, 5, 7, 9 and 10, the theorem is proved. □

Theorem 13. *For every connected graph G, $\eta(G) \neq 3$.*

Proof. By [5, Proposition 3], Lemma 2(i), Lemma 7, and Corollary 6, G has one – exactly one – non-complete block, say B. By Lemma 2(i), this block contains an induced subgraph H isomorphic to $K_4 - e$. Suppose that $H \neq B$. Since B does not have C_n, $n \geq 4$, as its induced subgraph, there exists $x \in V(B)$ such that x is adjacent to two vertices of H. Then the block B has either an induced subgraph isomorphic to C_4 or at least one induced subgraph isomorphic to $K_4 - e$ different from H. In each case, by Corollary 6 and Lemma 7, $\eta(G) \geq 4$, which is impossible. Thus $B = H$. From the block tree of G and Example 3, one can deduce that the vertices of degree 2 in H do not have a cut vertex in G. On the other hand, from Theorem 12, $G \in \mathcal{K}_2$, which is our final contradiction. □

We end this paper with the following example, which proves that for each non-negative integer $n \neq 1, 3$ there exists a graph G such that $\eta(G) = n$.

Example 14. Suppose that n is a non-negative integer different from 1 and 3. If G is a block graph, then by the Dobrynin–Gutman theorem $\eta(G) = 0$. It is clear that $\eta(K_4 - e) = 2$ and $\eta(C_5) = 5$. For an even integer $n > 2$, we construct a graph G from $K_4 - e$ such that $\eta(G) = n$. Suppose that G is yielding from $K_4 - e$ by adding $\frac{n-2}{2}$ edges to the vertex v_3 (or v_1); see the graph B depicted in Fig. 1. Then $\eta(G) = n$, as desired. If $n > 5$ is an odd integer, then we define the graph H to be constructed from C_5 by adding $\frac{n-5}{2}$ edges to a fixed vertex of C_5. Then $\eta(H) = n$, which completes our construction.

Acknowledgments

We are indebted to the referees for their suggestions and helpful remarks.

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